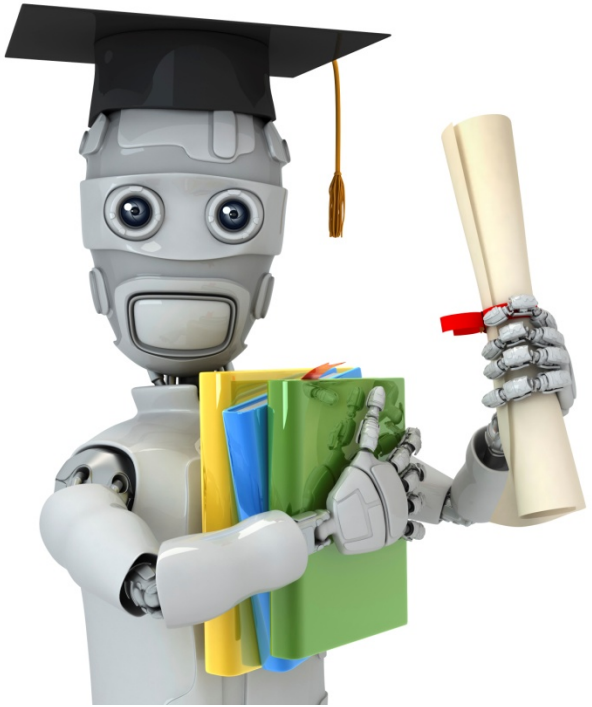


Machine Learning

Advice for applying machine learning

Deciding what to try next

Debugging a learning algorithm:

Suppose you have implemented regularized linear regression to predict housing prices.

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{j=1}^{m}\theta_j^2\right]$$

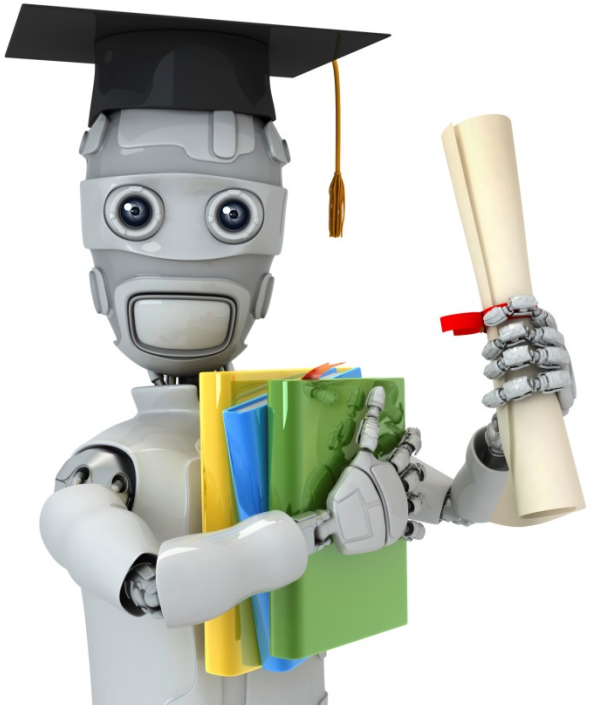
However, when you test your hypothesis on a new set of houses, you find that it makes unacceptably large errors in its predictions. What should you try next?

- Get more training examples
- Try smaller sets of features
- Try getting additional features
- Try adding polynomial features $(x_1^2, x_2^2, x_1x_2, \text{etc.})$
- Try decreasing λ
- Try increasing λ

Machine learning diagnostic:

Diagnostic: A test that you can run to gain insight what is/isn't working with a learning algorithm, and gain guidance as to how best to improve its performance.

Diagnostics can take time to implement, but doing so can be a very good use of your time.

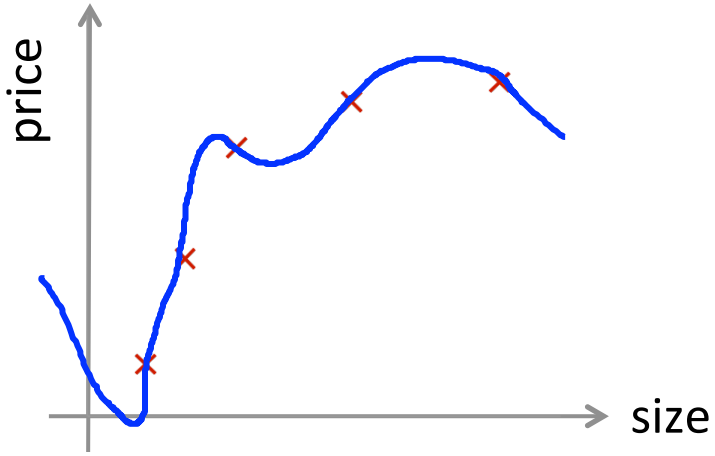


Machine Learning

Advice for applying machine learning

Evaluating a hypothesis

Evaluating your hypothesis



$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Fails to generalize to new examples not in training set.

$x_1 =$ size of house
$x_2 =$ no. of bedrooms
$x_3 =$ no. of floors
$x_4 =$ age of house
$x_5 =$ average income in neighborhood
$x_6 =$ kitchen size
$\vdots$
x_{100}

Evaluating your hypothesis

Dataset:

Size	Price
2104	400
1600	330
2400	369
1416	232
3000	540
1985	300
1534	315
1427	199
1380	212
1494	243

70%

Training set

30%

Test set

$(x^{(1)}, y^{(1)})$
$(x^{(2)}, y^{(2)})$
$\vdots$
$(x^{(m)}, y^{(m)})$

$(x_{test}^{(1)}, y_{test}^{(1)})$
$(x_{test}^{(2)}, y_{test}^{(2)})$
$\vdots$
$(x_{test}^{(m_{test})}, y_{test}^{(m_{test})})$

m_{test} = no. of test example

$(x_{test}^{(1)}, y_{test}^{(1)})$

Training/testing procedure for linear regression

- Learn parameter θ from training data (minimizing training error $J(\theta)$)

70%

- Compute test set error:

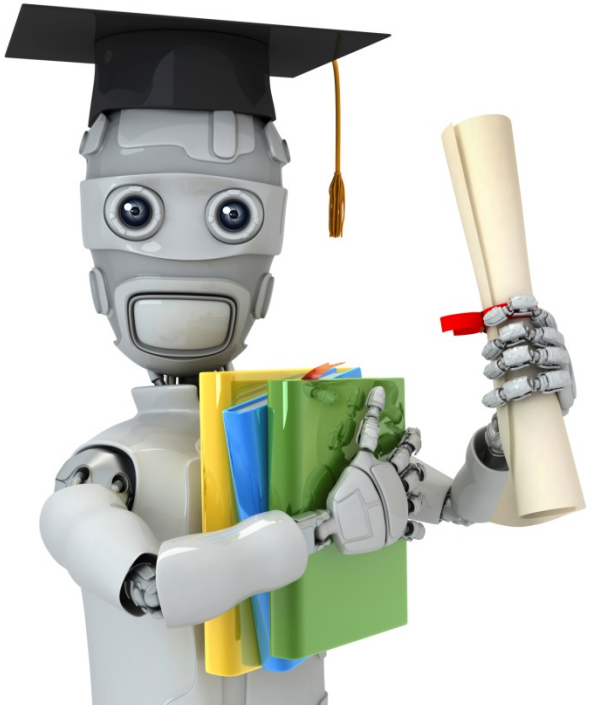
$$J_{test}(\theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} \left(h_\theta(x_{test}^{(i)}) - y_{test}^{(i)} \right)^2$$

Training/testing procedure for logistic regression

- Learn parameter θ from training data
- Compute test set error:

$$J_{test}(\theta) = -\frac{1}{m_{test}} \sum_{i=1}^{m_{test}} y_{test}^{(i)} \log h_\theta(x_{test}^{(i)}) + (1 - y_{test}^{(i)}) \log h_\theta(x_{test}^{(i)})$$

- Misclassification error (0/1 misclassification error):

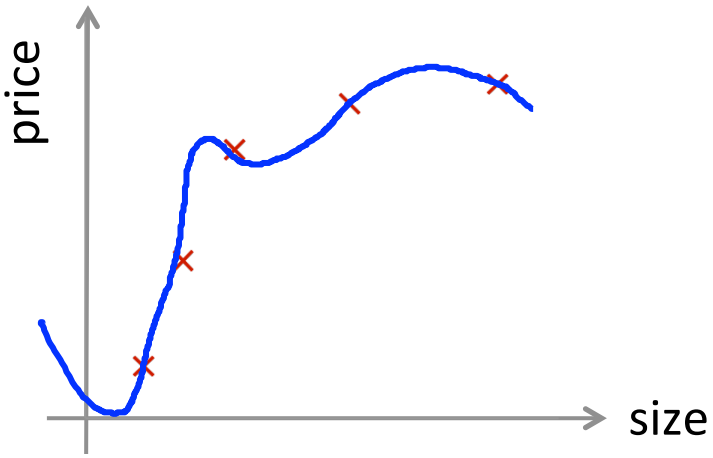


Machine Learning

Advice for applying machine learning

Model selection and training/validation/test sets

Overfitting example



$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

Once parameters $\theta_0, \theta_1, \ldots, \theta_4$ were fit to some set of data (training set), the error of the parameters as measured on that data (the training error $J(\theta)$) is likely to be lower than the actual generalization error.

Model selection

d = degree of polynomial

1. $h_\theta(x) = \theta_0 + \theta_1 x$ → $\theta^{(1)}$ → $J_{test}(\theta^{(1)})$
2. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$ → $\theta^{(2)}$ → $J_{test}(\theta^{(2)})$
3. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3$ → $\theta^{(3)}$ → $J_{test}(\theta^{(3)})$

⋮ ⋮

10. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$ → $\theta^{(10)}$ → $J_{test}(\theta^{(10)})$

Choose $\theta_0 + \ldots \theta_5 x^5$

How well does the model generalize? Report test set error $J_{test}(\theta^{(5)})$.

$\theta_0, \theta_1 \ldots$

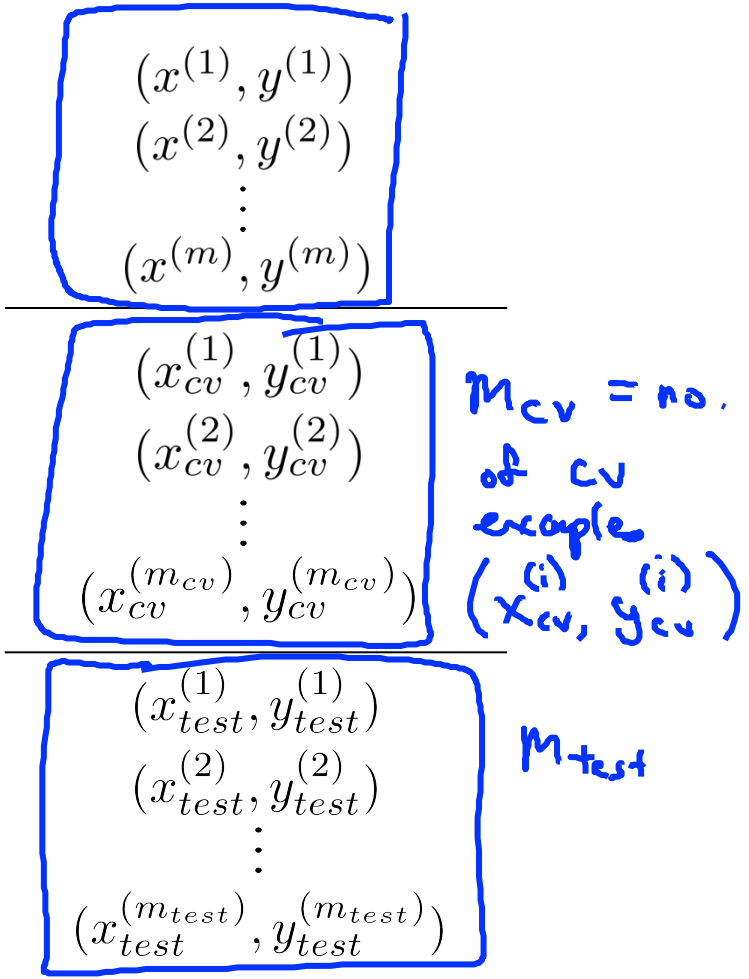
$\theta^{(5)}$

Problem: $J_{test}(\theta^{(5)})$ is likely to be an optimistic estimate of generalization error. I.e. our extra parameter (d = degree of polynomial) is fit to test set.

Evaluating your hypothesis

Dataset:

Size	Price	
2104	400	60% Training set
1600	330	
2400	369	
1416	232	
3000	540	
1985	300	
1534	315	20% Cross validation (CV) set
1427	199	
1380	212	20% test set
1494	243	



Train/validation/test error

Training error:

$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

$J(\theta)$

Cross Validation error:

$$J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$

Test error:

$$J_{test}(\theta) = \frac{1}{2m_{test}}\sum_{i=1}^{m_{test}}(h_\theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

Model selection

1. $h_\theta(x) = \theta_0 + \theta_1 x$ → $\min_\theta J(\theta)$ → $\theta^{(1)}$ → $J_{cv}(\theta^{(1)})$
2. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$ → $\theta^{(2)}$ → $J_{cv}(\theta^{(2)})$
3. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_3 x^3$ → $\theta^{(3)}$ → $J_{cv}(\theta^{(4)})$

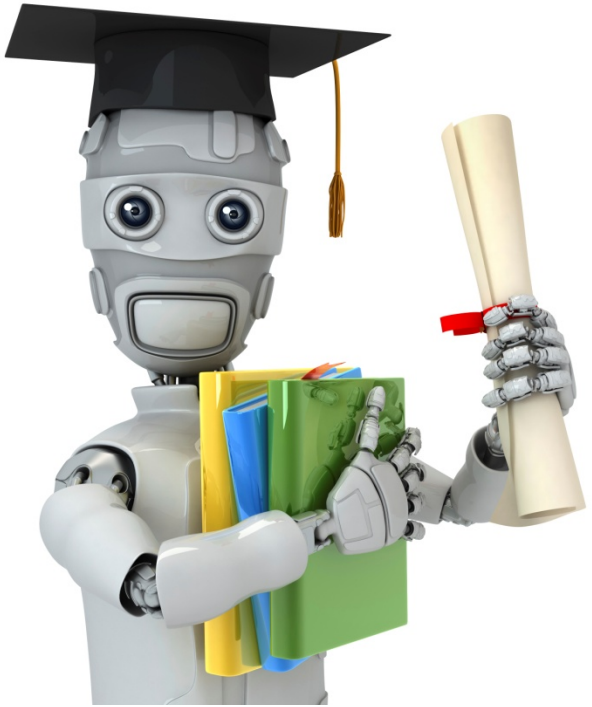
⋮

10. $h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}$ → $\theta^{(10)}$ → $J_{cv}(\theta^{(4)})$

$d = 4$

Pick $\theta_0 + \theta_1 x_1 + \cdots + \theta_4 x^4$

Estimate generalization error for test set $J_{test}(\theta^{(4)})$

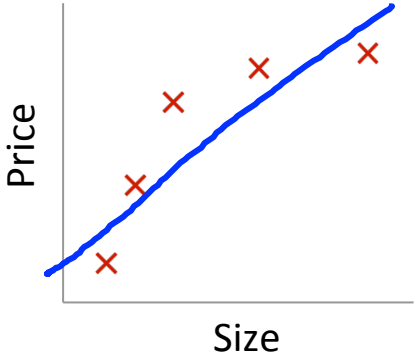


Machine Learning

Advice for applying machine learning

Diagnosing bias vs. variance

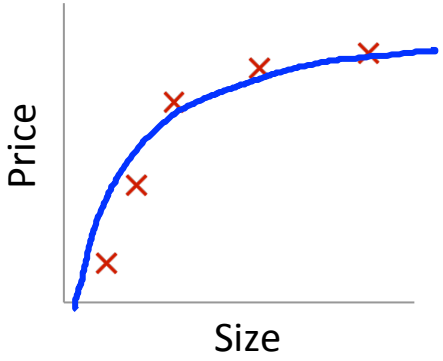
Bias/variance



$\theta_0 + \theta_1 x$

High bias
(underfit)

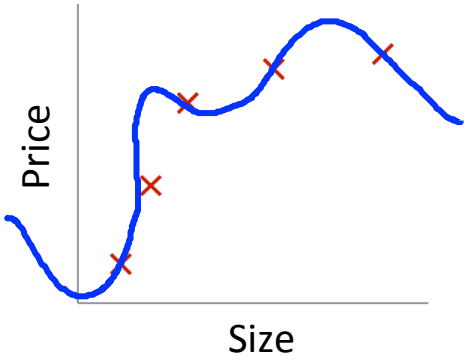
$d = 1$



$\theta_0 + \theta_1 x + \theta_2 x^2$

"Just right"

$d = 2$



$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

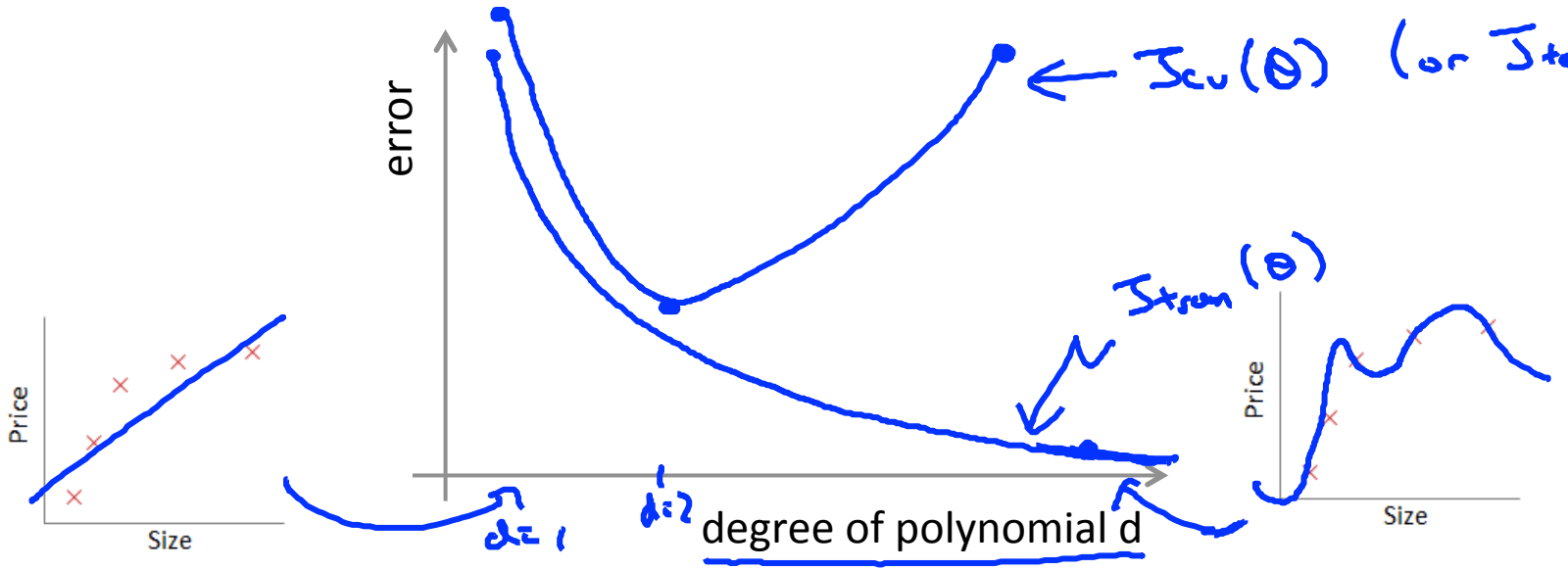
High variance
(overfit)

$d = 4$

Bias/variance

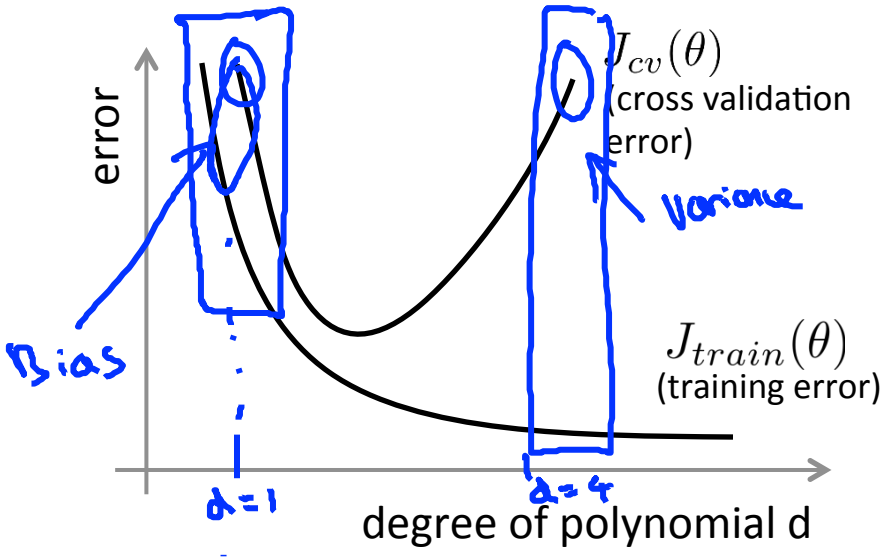
Training error: $J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$

Cross validation error: $J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$ (or $J_{test}(\theta)$)



Diagnosing bias vs. variance

Suppose your learning algorithm is performing less well than you were hoping. ($J_{cv}(\theta)$ or $J_{test}(\theta)$ is high.) Is it a bias problem or a variance problem?



Bias (underfit):

→ $J_{train}(\theta)$ will be high

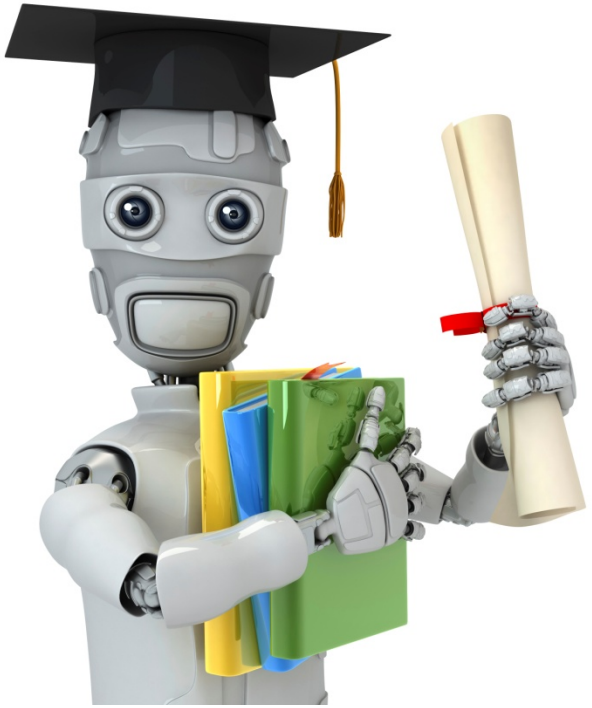
$J_{cv}(\theta) \approx J_{train}(\theta)$

Variance (overfit):

→ $J_{train}(\theta)$ will be low

$J_{cv}(\theta) \gg J_{train}(\theta)$

>>



Machine Learning

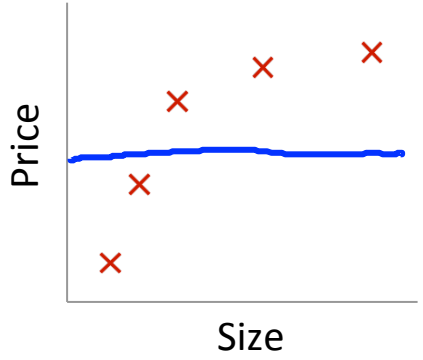
Advice for applying machine learning

Regularization and bias/variance

Linear regression with regularization

Model: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$$

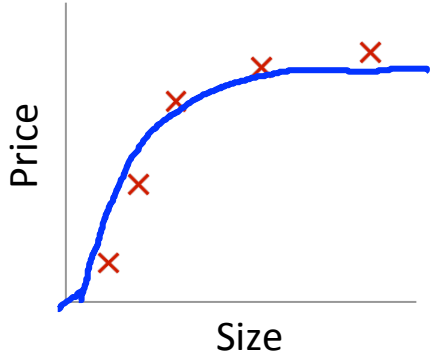


Large λ

→ High bias (underfit)

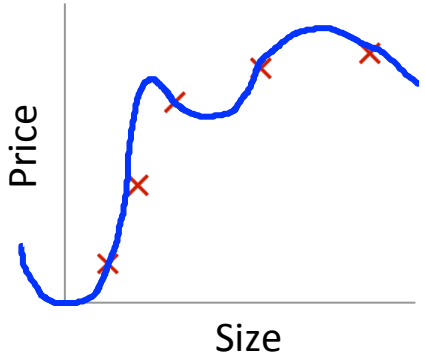
→ $\lambda = 10000.\ \theta_1 \approx 0, \theta_2 \approx 0, \ldots$

$h_\theta(x) \approx \theta_0$



Intermediate λ

"Just right"



→ Small λ

High variance (overfit)

→ $\lambda = 0$

Choosing the regularization parameter λ

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m} \sum_{j=1}^{m} \theta_j^2$$

$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

$$J_{cv}(\theta) = \frac{1}{2m_{cv}} \sum_{i=1}^{m_{cv}} (h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$

$$J_{test}(\theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_\theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

$J(\theta)$

J_{train}

J_{cv}

J_{test}

Choosing the regularization parameter λ

Model: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$$

1. Try $\lambda = 0$ → $\min_\theta J(\theta)$ → $\theta^{(1)}$ → $J_{cv}(\theta^{(1)})$
2. Try $\lambda = 0.01$ → $\min_\theta J(\theta)$ → $\theta^{(2)}$ → $J_{cv}(\theta^{(2)})$
3. Try $\lambda = 0.02$ → $\theta^{(3)}$ → $J_{cv}(\theta^{(3)})$
4. Try $\lambda = 0.04$
5. Try $\lambda = 0.08$ → $\theta^{(5)}$ $J_{cv}(\theta^{(5)})$

⋮

12. Try $\lambda = 10$ → $\theta^{(12)}$ → $J_{cv}(\theta^{(12)})$

0.24

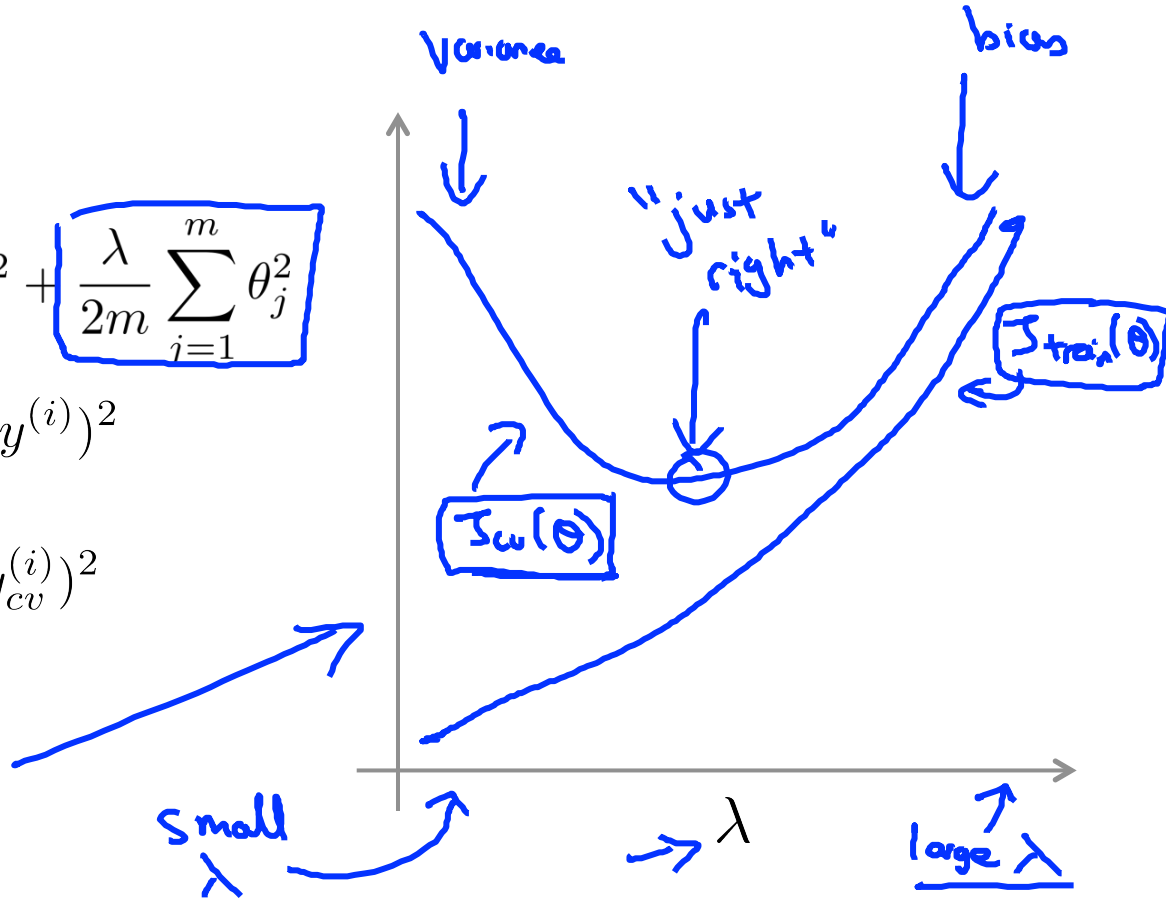
Pick (say) $\theta^{(5)}$. Test error: $J_{test}(\theta^{(5)})$

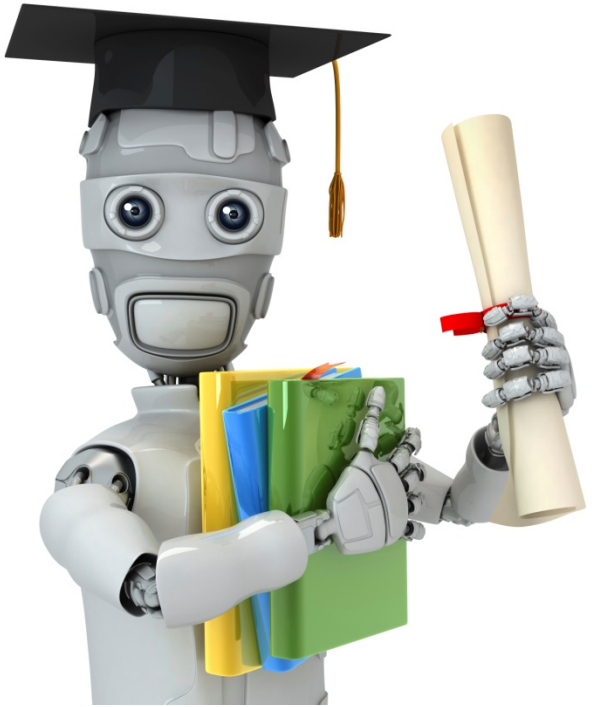
Bias/variance as a function of the regularization parameter λ

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{m}\theta_j^2$$

$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

$$J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$





Machine Learning

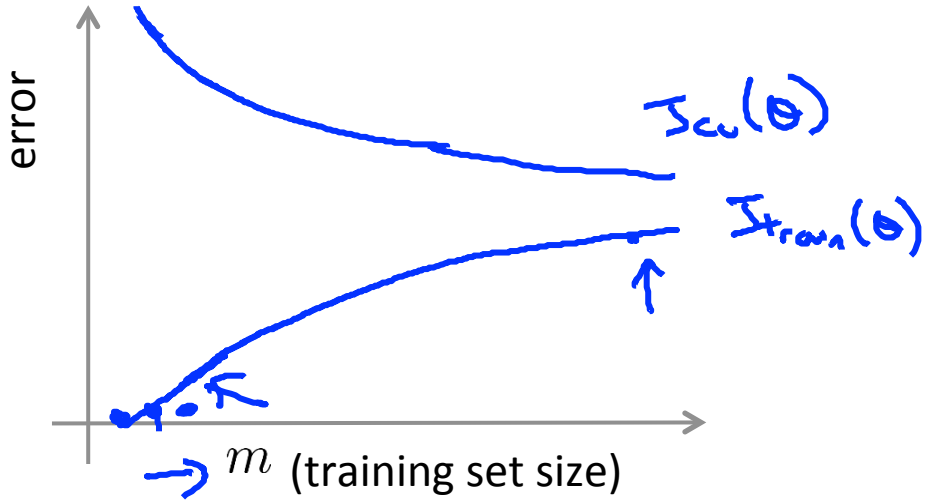
Advice for applying machine learning

Learning curves

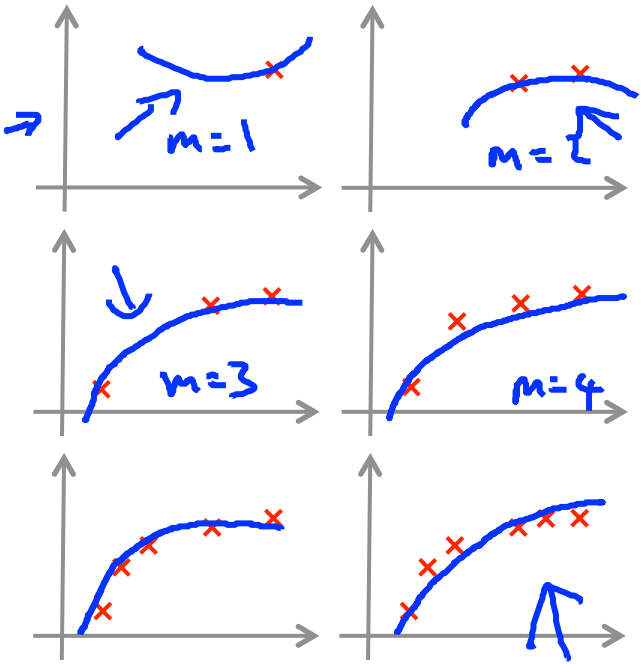
Learning curves

$$J_{train}(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

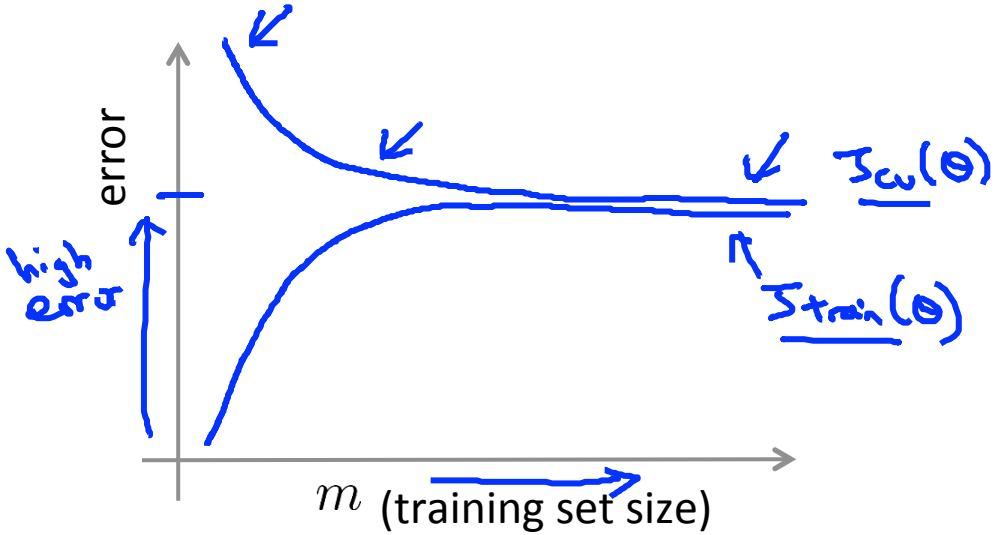
$$J_{cv}(\theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$



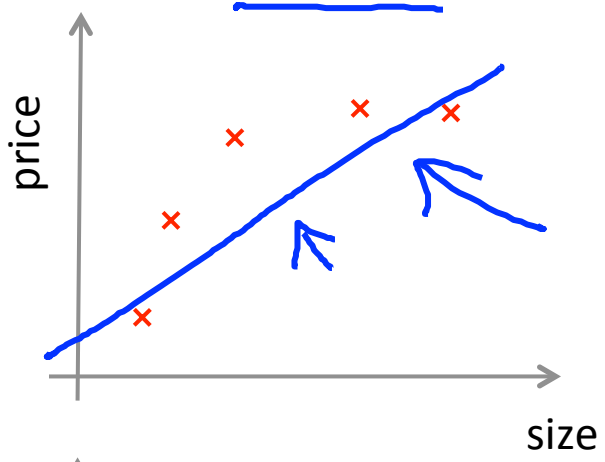
$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$

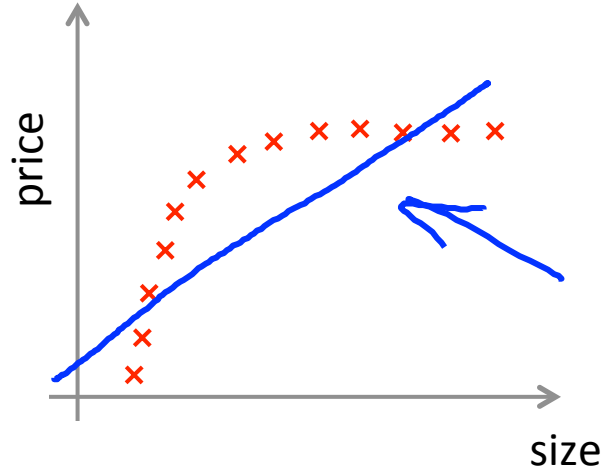


High bias



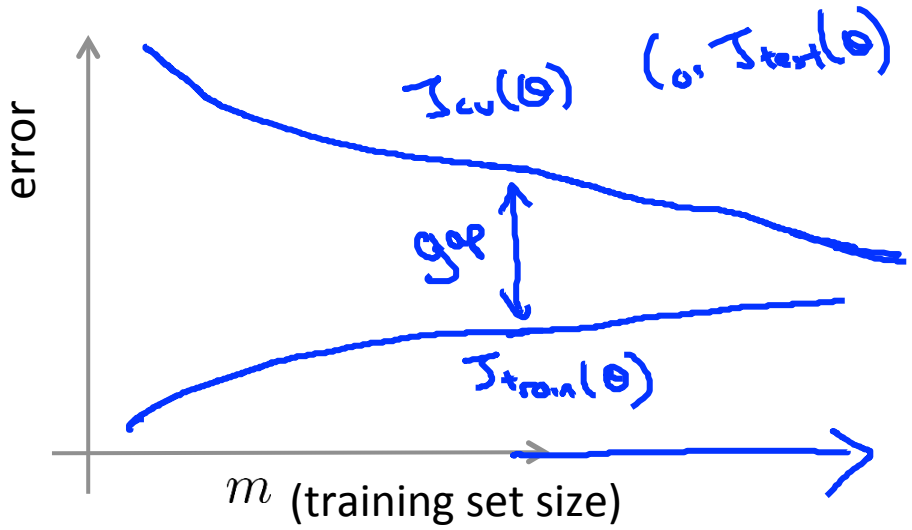
$h_\theta(x) = \theta_0 + \theta_1 x$





If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.

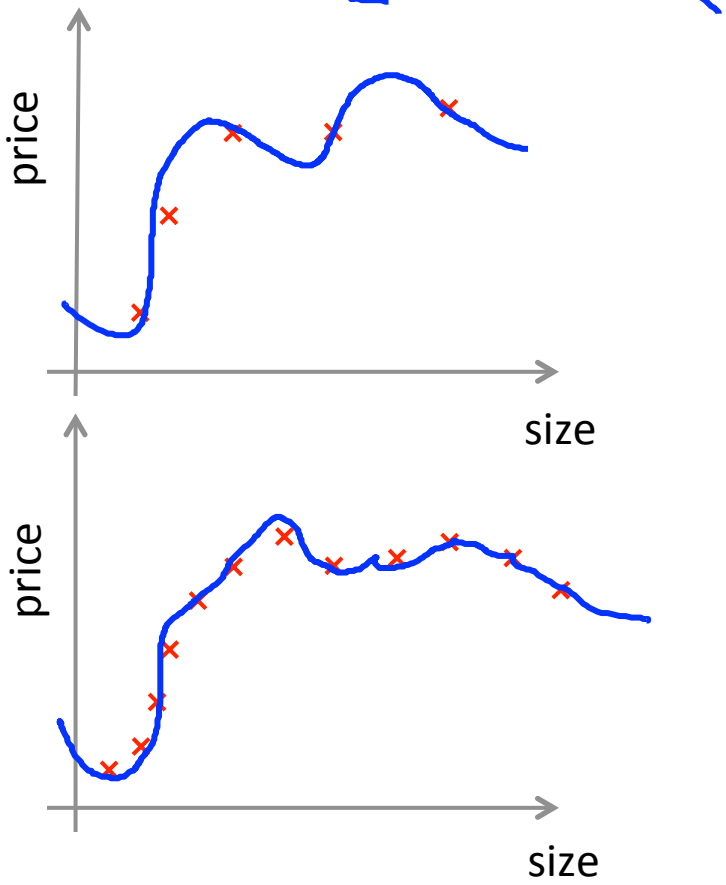
High variance

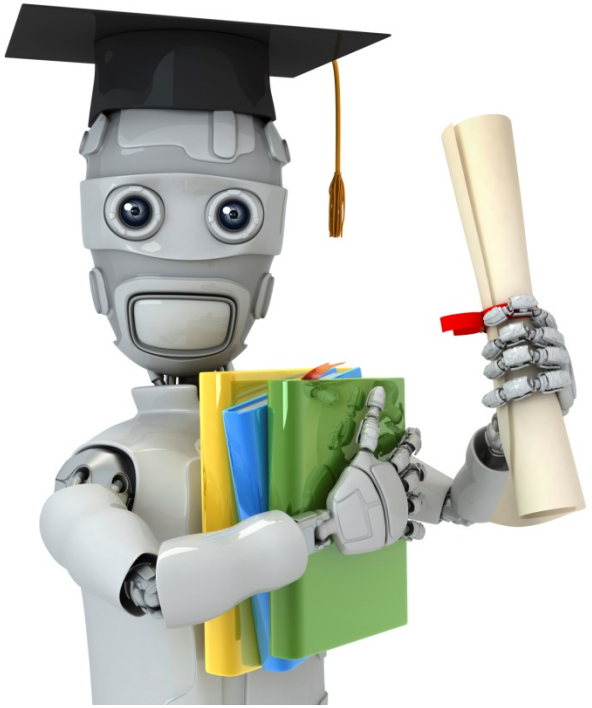


If a learning algorithm is suffering from high variance, getting more training data is likely to help.

$h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_{100} x^{100}$

(and small λ)





Machine Learning

Advice for applying machine learning

Deciding what to try next (revisited)

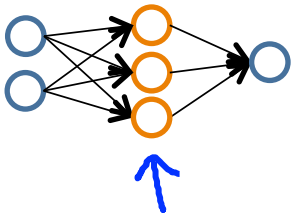
Debugging a learning algorithm:

Suppose you have implemented regularized linear regression to predict housing prices. However, when you test your hypothesis in a new set of houses, you find that it makes unacceptably large errors in its prediction. What should you try next?

- Get more training examples → fixes high variance
- Try smaller sets of features → fixes high variance
- Try getting additional features → fixes high bias
- Try adding polynomial features $(x_1^2, x_2^2, x_1x_2, \text{etc})$ → fixes high bias.
- Try decreasing λ → fixes high bias
- Try increasing λ → fixes high variance

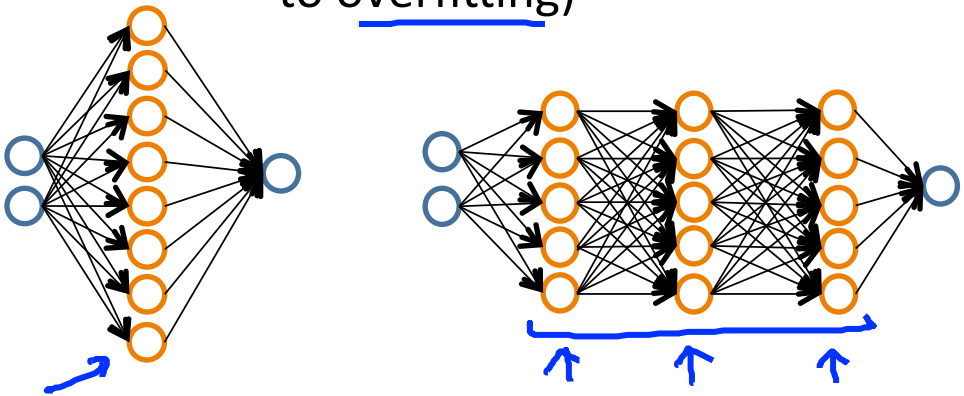
Neural networks and overfitting

"Small" neural network
(fewer parameters; more prone to underfitting)



Computationally cheaper

"Large" neural network
(more parameters; more prone to overfitting)



Computationally more expensive.

Use regularization (λ) to address overfitting.

$J_{cv}(\theta)$